

Phenyl salicylate

Other names:	2-Hydroxy-benzoic acid phenyl ester 2-Phenoxy carbonylphenol 2-hydroxybenzoic acid phenyl ester Benzoic acid, 2-hydroxy-, phenyl ester Fenylester kyseliny salicylove Musol NSC 33406 Phenol salicylate Phenyl 2-hydroxybenzoate Salicylic acid, phenyl ester Salol Salphenyl Seesorb 201 Seesorb K 201 phenyl 2-hydroxybenzenecarboxylate salicylic acid phenyl ester
Inchi:	InChI=1S/C13H10O3/c14-12-9-5-4-8-11(12)13(15)16-10-6-2-1-3-7-10/h1-9,14H
InchiKey:	ZQBAKBUEJOMQEX-UHFFFAOYSA-N
Formula:	C13H10O3
SMILES:	O=C(Oc1ccccc1)c1ccccc1O
Mol. weight [g/mol]:	214.22
CAS:	118-55-8

Physical Properties

Property code	Value	Unit	Source
chs	-6109.10	kJ/mol	NIST Webbook
gf	-105.14	kJ/mol	Joback Method
hf	-260.70	kJ/mol	Joback Method
hfus	26.08	kJ/mol	Joback Method
hvap	71.25	kJ/mol	Joback Method
log10ws	-3.15		Aqueous Solubility Prediction Method
logp	2.611		Crippen Method
mcvol	159.820	ml/mol	McGowan Method
pc	3862.67	kPa	Joback Method
rinpol	1650.00		NIST Webbook
rinpol	1702.00		NIST Webbook

rinpol	1655.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1702.00		NIST Webbook
rinpol	1650.00		NIST Webbook
tb	707.11	K	Joback Method
tc	962.79	K	Joback Method
tf	315.00 ± 1.50	K	NIST Webbook
tf	314.84 ± 0.20	K	NIST Webbook
tf	314.82 ± 0.20	K	NIST Webbook
tf	314.49 ± 0.20	K	NIST Webbook
tf	314.90	K	The use of organic calibration standards in the enthalpy calibration of differential scanning calorimeters
tf	314.53 ± 1.00	K	NIST Webbook
tf	314.83 ± 0.25	K	NIST Webbook
tt	314.75	K	Investigation of the melting behavior of the reference materials biphenyl and phenyl salicylate by a new type adiabatic scanning calorimeter
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.44	J/mol×K	707.11	Joback Method
cpg	425.94	J/mol×K	749.72	Joback Method
cpg	437.42	J/mol×K	792.34	Joback Method
cpg	448.02	J/mol×K	834.95	Joback Method
cpg	457.84	J/mol×K	877.56	Joback Method
cpg	467.02	J/mol×K	920.18	Joback Method
cpg	475.68	J/mol×K	962.79	Joback Method
dvisc	0.0000147	Paxs	707.11	Joback Method
dvisc	0.0001645	Paxs	512.01	Joback Method
dvisc	0.0000885	Paxs	551.03	Joback Method
dvisc	0.0003388	Paxs	472.99	Joback Method
dvisc	0.0000323	Paxs	629.07	Joback Method
dvisc	0.0000213	Paxs	668.09	Joback Method

dvisc	0.0000517	Paxs	590.05	Joback Method
hfust	19.20	kJ/mol	315.10	NIST Webbook
hfust	18.40 ± 0.50	kJ/mol	312.70	NIST Webbook
hfust	19.16	kJ/mol	315.00	NIST Webbook
hfust	18.98	kJ/mol	314.20	NIST Webbook
hsubt	109.10	kJ/mol	297.00	NIST Webbook
hvapt	69.90	kJ/mol	505.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	446.20	K	1.60	NIST Webbook

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1154.mol
Solubility of Salol in Pure Alcohols from (283.15 to 308.15) K: Crippen Method:	https://www.doi.org/10.1021/je800668j http://pubs.acs.org/doi/abs/10.1021/ci990307l
The use of organic calibration standards in the enthalpy calibration of Thermodynamic Study of Phenols: Salicylate Solutions in Aprotic Solvents At Different Temperatures: Aqueous Solubility Prediction Method:	https://www.doi.org/10.1016/j.tca.2012.03.028 https://www.doi.org/10.1021/je8003595 http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C118558&Units=SI
Investigation of the melting behavior of the reference materials biphenyl and phenyl salicylate by a new type adiabatic scanning calorimeter:	https://www.doi.org/10.1016/j.tca.2014.02.023 https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature

hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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